

Sparse solution of overdetermined linear systems when the columns of A are orthogonal

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Abstract

In this paper, we consider the problem of obtaining the best k -sparse solution of $Ax = y$ subject to the constraint that the columns of A are orthogonal. The naive approach for obtaining a solution to this problem has exponential complexity and there exist l_1 regularization methods such as Lasso to obtain approximate solutions. In this paper, we show that we can obtain an exact solution to the problem, with much less computational effort compared to the brute force search when the columns of A are orthogonal.

1 Introduction

We consider the following problem:

Problem 1 (P_1). *Find $u^k \in \mathbb{R}^n$ such that*

$$\|Au^k - y\| = \inf\{\|Ax - y\| \mid x \in \mathbb{R}^n, \|x\|_0 = k\}.$$

Here, the dimensions of u^k, A, y, x are $n \times 1, m \times n, m \times 1, n \times 1$ respectively, with $m > n$. Obtaining sparse solutions to overdetermined system of equations has a long history in the statistics community. For example, the Lasso algorithm due to Tibshirani ([Tibshirani(1996)]) tries to solve the following problem (for a fixed λ):-

$$\text{find } x \text{ such that } \|Ax - y\|_2^2 + \lambda\|x\|_1 \text{ is minimized}$$

l_1 norm is employed here rather than the l_0 as using l_1 penalization makes the problem tractable (convex optimization methods can be used to solve it) and also due to the fact that minimizing l_1 norm typically provides sparse solutions. The minimizer to the Lasso is obtained by solving a series of Quadratic Programming problems ([Tibshirani(1996)]). Other computational techniques also exist in the literature for solving the Lasso, e.g. see [Osborne et al.(2000a), Osborne et al.(2000b)].

The Lasso method is general and is applicable to any matrix. However, the parameter λ in the unconstrained formulation of the problem has to be tuned to obtain satisfactory results. λ is usually obtained by cross-validation.

Sparse solutions to overdetermined system are also considered in the paper by [Candes et al.(2005)]. The authors study the problem of reconstructing x exactly when the observed data are corrupted by noise. If

$$y = Ax + e$$

the authors give conditions on the matrix A and an minimizing algorithm which recovers x *exactly* subject to a constraint on the number of non-zero entries of e . However, this work is not directly relevant to the problem under consideration.

In this paper, we give an explicit solution to P_1 , under the constraint that the columns of A are orthogonal. We show that the solution given is equivalent (i.e. has equal error) to any solution obtained by a brute force search. One advantage of the method over the Lasso is that no tuning is necessary. As the proposed method still involves computing inverse of $A^T A$, it might not scale well to problems where n is very large.

2 Equivalence of solutions

We first fix some notation. If x is a vector let x_{\circ}^2 denote the element wise square of x . Let, $z = (A^T A)^{-1}(A^T y)_{\circ}^2$ and z_s be the result of sorting z (in a stable manner) in the decreasing order. Let f be a permutation such that $f(i) = j$ implies that $z_s(i) = z(j)$, where $x(i)$ denotes the i^{th} element of the vector x . Define, $x_{\text{pi}} = A^{\dagger} y$ and finally,

$$\begin{aligned} v^k(f^{-1}(i)) &= x_{\text{pi}}(f^{-1}(i)) \text{ if } i \leq k \\ v^k(f^{-1}(i)) &= 0, \text{ if } i > k \end{aligned}$$

Note here that v^k can be computed with much less computational effort than the brute force search as the inverse $(A^T A)^{-1}$ is only computed once.

Proposition 2.1. *Let A be an $m \times n$ matrix such that $m > n$, $n > 1$. Assume that A has full column rank. If the columns of A are orthogonal, then*

$$\|Au^k - y\| = \|Av^k - y\| \quad \forall y \in \mathbb{R}^m, \quad \forall k \in \{1, \dots, n\}$$

Proof. As u^k is a solution to P_1 , its non-zero elements should be of the form $u = (AC)^{\dagger} y$ where C is a $n \times k$ column picking matrix. Similarly, the non-zero

elements of v^k can be written as $v = RA^\dagger y$ where R is a $k \times n$ row picking matrix. We then have $\|Au^k - y\| = \|ACu - y\|$ and $\|Av^k - y\| = \|AR^T v - y\|$. Therefore,

$$\begin{aligned}
(ACu - y)^T(ACu - y) &= u^T C^T A^T ACu - 2y^T ACu + y^T y \\
&= y^T ((AC)^\dagger)^T C^T A^T AC(AC)^\dagger y - 2y^T AC(AC)^\dagger y + y^T y \\
&= -y^T AC(AC)^\dagger y + y^T y
\end{aligned} \tag{1}$$

$$\begin{aligned}
(AR^T v - y)^T(AR^T v - y) &= v^T RA^T AR^T v - 2y^T AR^T v + y^T y \\
&= y^T (A^\dagger)^T R^T RA^T AR^T RA^\dagger y - 2y^T AR^T RA^\dagger y + y^T y
\end{aligned} \tag{2}$$

Now, we prove that if the columns of A are assumed to be orthogonal i.e. if $A^T A$ is a diagonal matrix then $(ACu - y)^T(ACu - y) = (AR^T v - y)^T(AR^T v - y)$. To show this, we first try to find the C which minimizes $(ACu - y)^T(ACu - y)$. As has been shown above, this is equivalent to minimizing

$$-y^T AC(AC)^\dagger y + y^T y$$

or maximizing

$$(A^T y)^T C(C^T A^T AC)^{-1} C^T (A^T y) \tag{3}$$

As $A^T A$ is diagonal, $C(C^T A^T AC)^{-1} C^T = CC^T (A^T A)^{-1}$ and hence,

$$(A^T y)^T C(C^T A^T AC)^{-1} C^T (A^T y) = \sum_{i \in \{j | (CC^T)_{jj} \neq 0\}} \frac{(A^T y)_i^2}{\lambda_i} \tag{4}$$

where, λ_i 's are the diagonal elements of $A^T A$ (note that the λ_i 's are strictly positive real numbers). The maximum possible value of $\sum_{i \in \{j | (CC^T)_{jj} \neq 0\}} \frac{(A^T y)_i^2}{\lambda_i}$ is $\sum_{i \in \{j | (R^T R)_{jj} \neq 0\}} \frac{(A^T y)_i^2}{\lambda_i}$ as R picks the maximum k -components of $(A^T A)^{-1} (A^T y)_\circ^2$. So without loss of generality we can assume that $C = R^T$ as the error $\|ACu - y\|$ cannot be minimised any further.

The i^{th} row of the matrix $R^T RA^T A$ equals the i^{th} row of $A^T A$ if $R_{ii} = 1$ and equals the zero row otherwise. Therefore,

$$(A^T A)^{-1} R^T R(A^T A) R^T R(A^T A)^{-1} - 2R^T R(A^T A)^{-1} = -R^T R(A^T A)^{-1}$$

From $C = R^T$ we finally get

$$(A^T A)^{-1} R^T R(A^T A) R^T R(A^T A)^{-1} + C(C^T (A^T A) C)^{-1} C^T - 2R^T R(A^T A)^{-1} = 0$$

□

The above analysis raises the following question: can we say anything in the reverse? Supposing we are given that $\|Av^k - y\| = \|Au^k - y\|$ for all y , then is it true that the columns of A are orthogonal? We show below that this is indeed true for the case of $k = 1$. For the proof of this fact we need the following supporting lemma.

Lemma 2.1. *Let A be an $m \times n$ matrix such that $m > n$, $n > 1$. Assume that A has full column rank. If the diagonal entries of $(A^T A)^{-1}$ are inverses of the diagonal entries of $A^T A$ (i.e., if $(A^T A)_{ii}^{-1}(A^T A)_{ii} = 1$) then the off-diagonal elements of $A^T A$ (and hence the off-diagonal elements of $(A^T A)^{-1}$) are all equal to zero.*

Proof. First the claim is proved for $n = 2$ and the general case is proved by induction. For the case $n = 2$ assume that $A^T A = \begin{pmatrix} \alpha & \beta \\ \beta & \gamma \end{pmatrix}$ and $(A^T A)^{-1} = \begin{pmatrix} \frac{1}{\alpha} & \beta' \\ \beta' & \frac{1}{\gamma} \end{pmatrix}$. From,

$$\begin{pmatrix} \alpha & \beta \\ \beta & \gamma \end{pmatrix} * \begin{pmatrix} \frac{1}{\alpha} & \beta' \\ \beta' & \frac{1}{\gamma} \end{pmatrix} = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$$

we get that $\beta\beta' = 0$ and $\alpha\beta' + \frac{\beta}{\gamma} = 0$, which implies that $\beta = \beta' = 0$ proving the claim for this case. Now, we assume that the proposition is true for $n - 1$. Let

$$A^T A = \begin{pmatrix} \Sigma_{11} & \Sigma_{12} \\ \Sigma_{21} & \Sigma_{22} \end{pmatrix}$$

where Σ_{11} is an $(n-1) \times (n-1)$ matrix, Σ_{22} is a scalar, Σ_{12} is a $(n-1) \times 1$ vector and Σ_{21} is a $1 \times (n-1)$ vector. It is important to note here that $A^T A$ and Σ_{11} are symmetric positive definite matrices. Therefore, their inverses $(A^T A)^{-1}$ and Σ_{11}^{-1} are also symmetric and positive definite ([Harville(2008)], Corollary 14.2.11). Using blockwise matrix inversion, we can write $(A^T A)^{-1}$ as (see [Bernstein(2005)], p. 45)

$$\begin{pmatrix} \Sigma_{11}^{-1} + \Sigma_{11}^{-1}\Sigma_{12}(\Sigma_{22} - \Sigma_{21}\Sigma_{11}^{-1}\Sigma_{12})^{-1}\Sigma_{21}\Sigma_{11}^{-1} & -\Sigma_{11}^{-1}\Sigma_{12}(\Sigma_{22} - \Sigma_{21}\Sigma_{11}^{-1}\Sigma_{12})^{-1} \\ -(\Sigma_{22} - \Sigma_{21}\Sigma_{11}^{-1}\Sigma_{12})^{-1}\Sigma_{21}\Sigma_{11}^{-1} & (\Sigma_{22} - \Sigma_{21}\Sigma_{11}^{-1}\Sigma_{12})^{-1} \end{pmatrix}$$

Here, $(\Sigma_{22} - \Sigma_{21}\Sigma_{11}^{-1}\Sigma_{12})$ is the schur complement of Σ_{11} in $A^T A$ and is positive definite as $A^T A$ and Σ_{11} are both positive definite (see, [Boyd & Vandenberghe(2004)], Appendix A.5.5). Hence, the above blockwise matrix inversion formula is valid. Now, from

$$(\Sigma_{22} - \Sigma_{21}\Sigma_{11}^{-1}\Sigma_{12})^{-1} * \Sigma_{22} = 1$$

we get that $\Sigma_{21}\Sigma_{11}^{-1}\Sigma_{12} = \Sigma_{12}^T\Sigma_{11}^{-1}\Sigma_{12} = 0$. As Σ_{11}^{-1} is positive definite, we obtain that $\Sigma_{12} = 0$. Therefore,

$$(A^T A)^{-1} = \begin{pmatrix} \Sigma_{11}^{-1} & 0 \\ 0 & \Sigma_{22}^{-1} \end{pmatrix}$$

From the induction hypothesis we know that Σ_{11}^{-1} is a diagonal matrix. Therefore, $(A^T A)^{-1}$ is diagonal and the induction step is proved. \square

Proposition 2.2. *Let A be an $m \times n$ matrix such that $m > n$, $n > 1$. Assume that A has full column rank. Then,*

$$\|Au^1 - y\| = \|Av^1 - y\| \quad \forall y \in \mathbb{R}^m$$

if and only if the columns of A are orthogonal.

Proof. The forward implication has already been proved previously and to prove the reverse implication, we show the existence of a few y 's so that if expression if $\|Au^1 - y\| = \|Av^1 - y\|$ for all these choices of y then $A^T A$ is diagonal. We first choose $y = A(A^T A)^{-1}[1, 0, 0, \dots, 0]^T$ and look for solutions u^1 and v^1 .

For the above choice of y expression (3) reduces to:-

$$[1, 0, 0, \dots, 0]C(C^T A^T A C)^{-1}C^T[1, 0, 0, \dots, 0]^T$$

It is easy to see that the C which maximizes the above expression is $C = [1, 0, 0, \dots, 0]^T$ as for any other choice of C the expression equals zero.

Now, we shall show that

$$(A^T y)^T ((A^T A)^{-1} R^T R (A^T A) R^T R (A^T A)^{-1} - 2R^T R (A^T A)^{-1} + C(C^T (A^T A) C)^{-1} C^T) (A^T y) \quad (5)$$

can equal zero only for the choice $R = [1, 0, 0, \dots, 0]$. For this, let

$$A^T A = \begin{pmatrix} p_{11} & p_{12} & \cdots & p_{1n} \\ p_{21} & p_{22} & \cdots & p_{2n} \\ \vdots & \vdots & \cdots & \vdots \\ p_{n1} & p_{n2} & \cdots & p_{nn} \end{pmatrix}, (A^T A)^{-1} = \begin{pmatrix} j_{11} & j_{12} & \cdots & j_{1n} \\ j_{21} & j_{22} & \cdots & j_{2n} \\ \vdots & \vdots & \cdots & \vdots \\ j_{n1} & j_{n2} & \cdots & j_{nn} \end{pmatrix}$$

When $R = [1, 0, 0, \dots, 0]$ we get that the value of expression (5) is equal to $p_{11}j_{11}^2 - 2j_{11} + \frac{1}{p_{11}}$. This value can be made zero by choosing $j_{11} = \frac{1}{p_{11}}$. For any other choice of R such that $R_i = 1, i \neq 1$, the value of expression (5) is equal to $p_{ii}j_{ii}^2 + \frac{1}{p_{ii}}$. This value cannot be made zero by any choice of j_{ii} as $p_{ii} > 0$. As expression (5) has to equal zero from our initial assumption, we are forced to choose $j_{11} = \frac{1}{p_{11}}$.

Now, we choose $y = A(A^T A)^{-1}[0, 1, 0, \dots, 0]^T$ and obtain that $j_{22} = \frac{1}{p_{22}}$. By continuing in this fashion, we get that $j_{ii} = \frac{1}{p_{ii}} \quad \forall i \in \{1, 2, 3, \dots, n\}$. Finally, we apply Lemma 2.1 and get that both $A^T A$ and $(A^T A)^{-1}$ are diagonal. \square

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